

AD-A191 489

STUDY OF MIXING AND REACTION IN THE FIELD OF A VORTEX

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(U) CALIFORNIA UNIV IRVINE DEPT OF MECHANICAL
ENGINEERING B M CETEGEN ET AL

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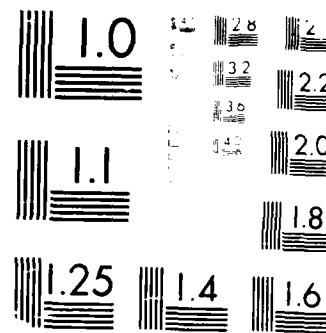
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REPORT DOCUMENTATION PAGE

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1a. REPORT SECURETY Unclassified	1b. RESTRICTIVE MARKINGS None			
2a. SECURITY CLASSIFICATION AUTHORITY Unclassified	3. DISTRIBUTION/AVAILABILITY OF REPORT Distribution unlimited; approved for public release			
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE Unclassified	4. PERFORMING ORGANIZATION REPORT NUMBER(S) S-IC SELECTED MAR 15 1988			
5a. NAME OF PERFORMING ORGANIZATION University of California Dept. of Mechanical Engr.	5b. OFFICE SYMBOL (If applicable) S-CD	7a. NAME OF MONITORING ORGANIZATION Air Force Office of Scientific Research		
6c. ADDRESS (City, State and ZIP Code) Irvine, CA 92717	7b. ADDRESS (City, State and ZIP Code) Bolling AFB DC 20332-6448			
8a. NAME OF FUNDING SPONSORING ORGANIZATION Air Force Office of Sci. Res.	8b. OFFICE SYMBOL (If applicable) AFOSR/NA	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER HAFOSR-86-0016		
10. SOURCE OF FUNDING NOS Bolling AFB DC 20332-6448	PROGRAM ELEMENT NO 61102F	PROJECT NO 2308	TASK NO A2	WORK UNIT NO
11. TITLE (Include Security Classification) Study of Mixing and Reaction in the Field of a Vortex	12. PERSONAL AUTHOR(S) B.M. Cetegen and W.A. Sirignano			
13a. TYPE OF REPORT Publication	13b. TIME COVERED FROM 10/86 TO 10/87	14. DATE OF REPORT (Yr. Mo. Day) November 20, 1987	15. PAGE COUNT 3	
16. SUPPLEMENTARY NOTATION				
17. COSATI CODES FIELD GROUP SUB GR	18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number) Turbulent Reacting Flows; Molecular Mixing and Reaction in Turbulent Structures			
19. ABSTRACT (Continue on reverse if necessary and identify by block number) In turbulent reacting flows, completion of chemical reactions requires diffusion of reactive species at a molecular level. Eddies rich in one reactant can be present in many turbulent flows involving finite rate chemical reactions. Local species stratifications are dissipated by molecular diffusion and chemical reaction under the influence of the local flow field. In many turbulent flows, the local flow field has a strong rotational character. It is mostly this rotational motion which enhances mixing through flow stretch and convection leading to mixing at the molecular level. In this paper, molecular mixing and finite rate chemical reactions in a two dimensional viscous vortex are examined analytically. Two species initially separated across a plane are allowed to diffuse and react in the presence of a line vortex centered at this separation plane. Concentration fields and the probability density functions (pdf) are determined for a range of vortex strengths and for several values of Schmidt number				
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT <input checked="" type="checkbox"/> DTIC USERS <input checked="" type="checkbox"/>		21. ABSTRACT SECURITY CLASSIFICATION Unclassified		
22a. NAME OF RESPONSIBLE INDIVIDUAL Julian M. Tishkoff		22b. TELEPHONE NUMBER (Include Area Code) (202) 767- <u>3465</u>	22c. OFFICE SYMBOL AFOSR/NA	

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE

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STUDY OF MIXING AND REACTION IN THE FIELD
OF A VORTEX*

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Abstract

In turbulent reacting flows, completion of chemical reactions requires diffusion of reactive species at a molecular level. Eddies rich in one reactant can be present in many turbulent flows involving finite rate chemical reactions. Local species stratifications are dissipated by molecular diffusion and chemical reaction under the influence of the local flow field. In many turbulent flows, the local flow field has a strong rotational character. It is mostly this rotational motion which enhances mixing through flow stretch and convection leading to mixing at the molecular level.

In this paper, molecular mixing and finite rate chemical reactions in a two dimensional viscous vortex are examined analytically. Two species initially separated across a plane are allowed to diffuse and react in the presence of a line vortex centered at this separation plane. Concentration fields and the probability density functions (pdf) are determined for a range of vortex strengths and for several values of Schmidt number at different times during the growth of the vortex. Finite rate isothermal chemical reactions are also considered. The results for the reacting vortex are compared with those for the nonreacting vortex and some insight is gained concerning the form of the pdf in such configurations.

Method of Analysis

Nonreacting Vortex

The concentration field within a nonreacting viscous line vortex imposed coincident with an interface separating the two species is calculated by analyzing the local behavior in a Lagrangian frame of reference. Computation of the successive locations of a material element starting from its initial position is achieved by integration of the flow field with respect to time. In this study, the analytical solution for the flowfield of a viscous line vortex⁽¹⁾ is utilized. Across the

material surface separating the two species, molecular diffusion takes place as this interface is stretched and transported in the vortex flow field. The local concentration distribution around interfaces can be obtained analytically. Until this point, the analysis generally follows References 2 and 3. In the solution for the concentration field within the vortex, the concentration at a given location is composed from superposition of analytical solutions. Concentrations at many locations are obtained and used to construct the pdfs assuming periodicity of the vortices and utilizing Taylor's frozen flow assumption.

Chemically Reacting Vortex

In case of finite rate chemical reactions within the vortex, an approximate method based on Green's function solution of the reacting species conservation equation is implemented. Solution for the mass fraction of one reactive species, together with the solution for the appropriate Shvab-Zel'dovich variable, allows determination of both fuel and oxidizer distributions within the vortex.

In this paper, a dilute isothermal reaction between NO and O₃ is considered. The reaction products are NO₂ and O₂ and both reactants are diluted in N₂. The mass fractions far from the vortex are taken to be 0.01 for both reactants. The second order reaction rate was taken from Givi, et al⁽⁴⁾.

Detailed description of the analyses for nonreacting and chemically reacting vortices can be found in Reference (5).

Results

The first four figures present results for the nonreacting case. Of course, they also apply to the passive scalar in the reacting case. Figure 1a shows the distortion of an initially horizontal material line located along the x axis at a certain instant after the vortex initiation for a nondimensional vortex strength (Re = $\Gamma/2\pi\nu$) of 50. The initial concentration field corresponds to the upper half plane of

* This work was supported by an AFOSR grant.

concentration 0.0 and the lower half plane of concentration 1.0. The computed concentration profiles in the x direction at different y locations show a well-mixed core region surrounded by concentration variations in the outer regions and the arms of the vortex for Schmidt number of unity. The character of the concentration profiles for large Schmidt numbers, typical of liquids, is considerably different showing sharp variations of concentration between adjacent stratifications within the vortex which have not diffused because of the low molecular diffusivity. The pdfs constructed from such concentration profiles are shown in Figures 2, 3, and 4 to delineate the effects of vortex strength, Schmidt number and time.

Figure 2 shows the pdf as a function of the concentration and normalized transverse distance for two vortex strengths at a given time and $Sc = \nu/L$ of unity. The length scale chosen to normalize the transverse distance approximately accounts for the growth of the vortex with time and its dependence on the vortex strength. Therefore, the normalized coordinates $\tilde{x} = x/\sqrt{4\pi t} Re$ and $\tilde{y} = y/\sqrt{4\pi t} Re$ are convenient in presentation of results. The probability density function shows two peaks at the unmixed concentrations outside the mixing region. Probabilities at intermediate concentrations develop as a result of mixing by molecular diffusion and vortex interaction. As the vortex strength increases, the probability of the concentrations in the mid-range (0.4 - 0.6) increases in the core of the vortex. The peaks at $\tilde{y} > 0$ for $C > 0.5$ and those at $\tilde{y} < 0$ for $C < 0.5$ are results of the vortex motion bringing the high concentrations from lower plane to the upper and vice versa. The counterclockwise vortex motion is also apparent in these pdfs. The continuing line of peaks on each side joining to the peaks at $C = 0.0$ and $C = 1.0$ result from diffusive regions around the interfaces. The shapes of the pdfs are similar to those computed in shear layers. It also resembles the qualitative features of the experimentally determined pdfs in shear layers.

Figure 3a and 2b shows the time evolution of pdf at a vortex strength of $Re = 50$. At early time instant, the probabilities of intermediate concentrations are small and in fact the shapes of the probability peaks at the minimum and maximum concentrations are similar to those observed for the high Schmidt number case shown in Figure 4. At a later instant, the effect of the vortex becomes more pronounced and the higher probabilities of mixing appear in the center of the vortex.

Figure 4 shows the probability densities at large Schmidt numbers typical of liquids. These pdfs are characterized by two peaks at the unmixed concentrations with a minute amount of mixing in the core region. The shapes of the probability peaks can be approximately correlated by the length scale chosen in the transverse direction. These pdfs also resemble the earlier time pdf for Schmidt number of unity.

One convenient measure of molecular mixing can be defined in terms of the probabilities and concentrations as:

$$f = \frac{1}{2L} \int_{-L}^{+L} [1 - 4 \int_0^1 P(C, y) (C - 0.5)^2 dC] dy \quad (1)$$

In this expression, $P(C)$ is the normalized probability. This parameter can be referred to as "mixedness" and its values range from zero for no

mixing ($C = 0$ or 1 only) to unity for complete mixing ($C = 0.5$ everywhere). The values of this parameter were computed for a range of values of vortex strengths ($Re = 10-500$) and Schmidt number ($Sc = 1-1000$). In these calculations, $2L$ was taken to cover the whole extent of the largest vortex considered here ($L = 10.0$). Empirical correlation of the computed mixing factors suggests an expression given by,

$$f = 0.8 Sc^{-1/2} \left[\frac{4\pi t}{L^2} \right]^{1/2} + 0.1 Re \left[\frac{4\pi t}{L^2} \right]^{1/2} \quad (2)$$

The "mixedness" increases continuously with increasing vortex strength. The mixing at zero Reynolds number limit, the first term, corresponds to a diffusion layer growing in the y direction with time. The second term is the mixing enhancement by the vortex. Current results indicate that the enhancement factor is linear in Re . However, there appears to be negligible dependence of this factor on Schmidt number.

Figures 5a and 5b show the concentration distributions in the (\tilde{x}, \tilde{y}) plane for nonreacting and reacting vortices of a nondimensional strength of 50. The nonreacting vortex is characterized by a well-mixed core around $C = 0.5$ and the diffusive regions surrounding the core and the vortex arms. The vortex with finite rate chemical reactions has a considerably different character. As expected, the reactive species has been depleted in the core region. Around the core, the spatial mass fraction gradients appear to be steeper than the nonreacting vortex. Below the vortex center, a tongue of unreacted species is observed. This region corresponds to the zone between the outer arm of the vortex and the core where one reactant is abundant.

The corresponding pdfs are shown in Figures 3a and 3b. Figure 3a displays the typical features of nonreacting vortex pdf at early times. In comparing the two pdfs, the reacting vortex pdf does not contain the vortex core peaks and the effect of the reacted core on the pdf appears as modification of the probability peak topography at $C = 0.0$. The new probability peak at $C = 0.0$ near the vortex center corresponds to the reacted core region.

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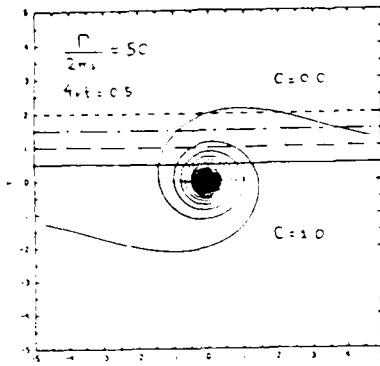
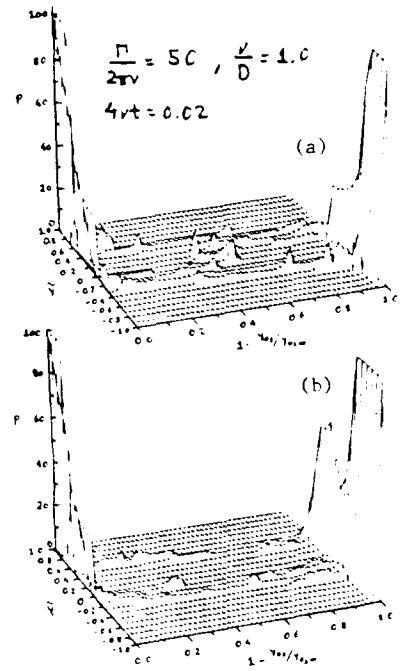


Figure 1. Distortion of a horizontal material line by a viscous line vortex.



(a)

(b)

Figure 3. Comparison of pdfs for nonreacting (a) and reacting (b) scalars at $Re = 50$, $4vt = 0.02$, $Sc = 1.0$.

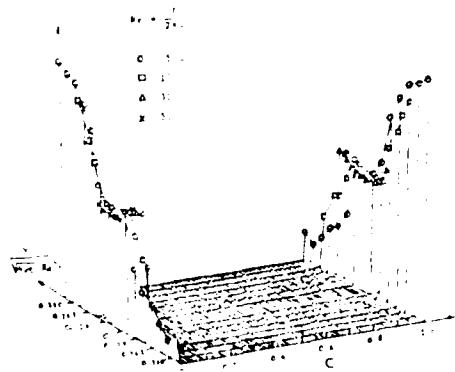


Figure 4. Pdf at a range of vortex strengths at $Sc = 1.0$.

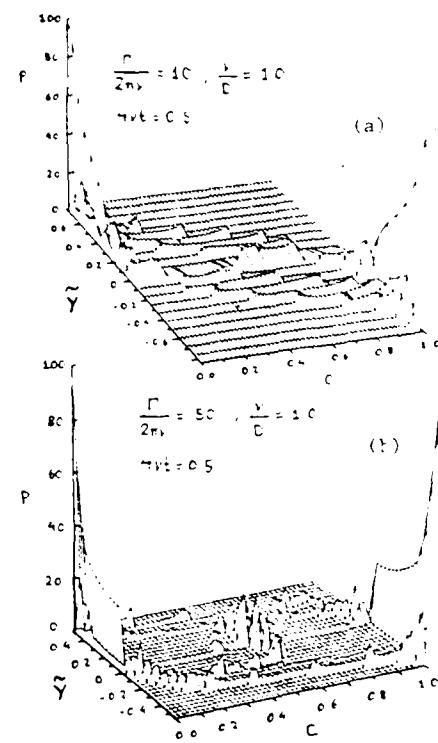


Figure 2. Effect of vortex strength on the pdf of a nonreacting scalar for $Sc = 1.0$.

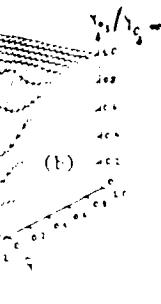
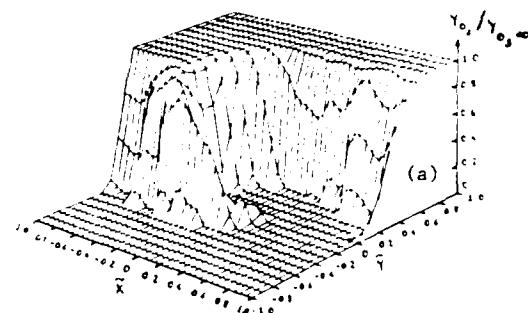


Figure 5. Concentration profiles for nonreacting (a) and reacting (b) species at $Re = 5$, $\nu/D = 1.0$, $Sc = 1.0$.

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